

Research Paper

State Space Model Predictive Control of a Reactive Distillation Process

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Abstract: *This work has been carried out to demonstrate the performances of four different state space models in the model predictive control system of a reactive distillation process that was used for the production of ethyl acetate. The state space models of the reactive distillation process were developed with the aid of System Identification Toolbox of MATLAB using the data acquired from the reactive distillation column set up. The control algorithms were developed and simulated in MATLAB environment with the aid of Model Predictive Control Toolbox. The top segment, the reaction segment and the bottom segment temperatures were selected as the controlled variables while the reflux ratio, the feed ratio and the reboiler duty were respectively chosen as the manipulated variables. Compared to the other state space model predictive controllers investigated, the best closed-loop dynamic responses with the smallest number of oscillations, fastest rise time and fastest response time obtained from n4sid state space model predictive controller showed that it had the best performance. Further simulations of the n4sid state space model predictive controller for mismatch revealed that it was very robust as the mismatch only affected the performance of the controller very slightly.*

Keywords: Model predictive control, state space models, reactive distillation process, ethyl acetate, MATLAB.

1. Introduction:

Reactive distillation is very attractive whenever conversion is limited by reaction equilibrium (Balasubramhanya and Doyle III, 2000) because it combines the benefits of equilibrium reaction with distillation to enhance conversion provided that the product of interest has the largest or the lowest

boiling point (Taylor and Krishna, 2000). It has a lot of advantages which include reduced investment and operating costs, environmental impacts, and so on, due to increased yield of a reversible reaction by separating the product of interest from the reaction mixture (Pérez-Correa *et al.*, 2008), higher conversion, improved selectivity, lower energy consumption, scope for difficult separations and avoidance of azeotropes (Jana and Adari, 2009).

However, due to the integration of reaction and separation, reactive distillation exhibits complex behaviors (Khaledi and Young, 2005), such as steady state multiplicity, process gain sign changes (bidirectionality) and strong interactions between the process variables (Jana and Adari, 2009). These complexities have made the modeling as well as the control of the reactive distillation process extremely difficult. Thus, the development of a high performance and robust control algorithm for this process is still a challenge to chemical engineers. A proposed strategy for the control of a system like this (in which there are significant interactions between the loops and in which there exist complex and unusually problematic dynamics (such as long time delays, and inverse response, or even unusually large time constants)) is "Model Predictive Control (MPC)".

Model predictive control is an important advanced control technique for difficult multivariable control problems (Seborg *et al.*, 2004). Its primary advantage is the explicit handling of constraints (Bequette, 2003). In model predictive control, as the name implies, a model is used. This model can have variety of forms which include theoretical dynamic models, neural network dynamic models, transfer function models, and state space models. However, no matter the form of the models being used, when the model predictive control algorithm is to implement the control action, the models are normally linearized, if nonlinear, because model predictive control requires the model to be linear, time invariant (LTI). As an alternative, for a nonlinear system/process, a very common method is to linearize the control model and/or plant model before using it in the model predictive control algorithm. One of the ways of representing a nonlinear process as a linear one is the use of state space models. Apart from the use of state space models in the model predictive control of reactive distillation process considered in this work, many methods have been used in the literature for the control of this process.

Sneesby *et al.* (1997) worked on the dynamic simulation and control of reactive distillation for the synthesis of ethyl tert-butyl ether and presented general recommendations for the control of the reactive column of this type. Bock *et al.* (1997) developed a control structure for a reactive column with a recovery column by analysing the reaction column's steady state and dynamic sensitivity of possible disturbances and manipulated variables. Sneesby *et al.* (1999) used an ethyl tert-butyl ether reactive distillation column as a case study to show how a two-point control configuration, which recognized the importance of both composition and conversion, can be developed and implemented for a reactive distillation process. Kumar and Daoutidis (1999) studied the dynamic behaviour and control of an ethylene glycol reactive distillation column by deriving a detailed tray-by-tray model that explicitly included the vapor-phase balances. Monroy-Loperena *et al.* (2000) studied the control problem of an ethylene glycol reactive distillation column with the control objective of regulating the ethylene glycol composition in the product by manipulating the reboiler boil-up ratio. Al-Arfaj and Luyben (2000) explored the closed-loop control of a reactive distillation column with two products and discovered that single-end temperature control could keep both products at or above specified purity values, even for large disturbances, if reactive-zone holdup was sufficiently large. Vora and Daoutidis (2001) studied the dynamics and control of an ethyl acetate reactive distillation system and designed model-based linear and nonlinear state feedback controllers, along with conventional SISO PI controllers. Khaledi and Young (2005) investigated the nonlinearity of an ethyl tert-butyl ether reactive distillation column and developed a 2 x 2 unconstrained model predictive control scheme for product purity and reactant conversion control by using the process dynamics approximated by a first-order plus dead time model to estimate the process model for the model predictive controller. Völker *et al.* (2007) designed a multivariable controller for a medium-scale semi-batch reactive distillation column and showed experimentally that the controller performed well for large set-point changes and in the face of process disturbances. Grüner *et al.* (2003) applied asymptotically exact input/output-linearization to an industrial reactive distillation column and found that in comparison with a well-tuned linear controller, the controller showed a superior performance with respect to set-point

changes and disturbances, even in the presence of unknown input delays. Giwa and Karacan (2012e) used neural network and transfer function models as the controller models to demonstrate the decoupling model predictive control of a reactive packed distillation column for the production of ethyl acetate.

In this work, representing the process dynamics using different forms of state space models, the model predictive control of ethyl acetate reactive distillation process (RDP) was accomplished for set-point tracking.

2. Procedures:

2.1 Data Acquisition:

The data used for the development of the state space models used in this work was generated from a reactive distillation column set-up as shown in Figure 1a (pictorially) and b (schematically). The equipment set-up was also described in the researches of Giwa and Karacan (2012a, 2012b, 2012c, 2012d and 2012e). The column, excluding the condenser and the reboiler, had a height of 1.5 m and a diameter of 0.05 m. It consisted of a cylindrical condenser of a diameter and a height of 5 and 22.5 cm respectively. The main column section of the plant was divided into three subsections of 0.5 m each. The upper, middle and lower sections were the rectifying, the reaction and the stripping sections respectively. The rectifying and the stripping sections were packed with raschig rings while the reaction section was filled with Amberlyst 15 solid catalyst that had a surface area of 5300 m²/kg, a total pore volume of 0.4 cc/g and a density of 610 kg/m³. The reboiler was spherical in shape with a volume of 3 Litre. The column was fed with acetic acid at the top (between the rectifying section and the reaction section) while ethanol was fed at the bottom (between the reaction section and the stripping section) with the aid of peristaltic pumps which were operated with the aid of a computer via MATLAB/Simulink program. All the signal inputs (reflux ratio, feed ratio and reboiler duty) to the column and the measured outputs (top segment temperature, reaction segment temperature and bottom segment temperature) from the column were sent and recorded respectively on-line with the aid of MATLAB/Simulink computer program and electronic input-output (I/O) modules that were connected to the equipment and the computer system. The esterification reaction occurring in the column was an equilibrium type given as:

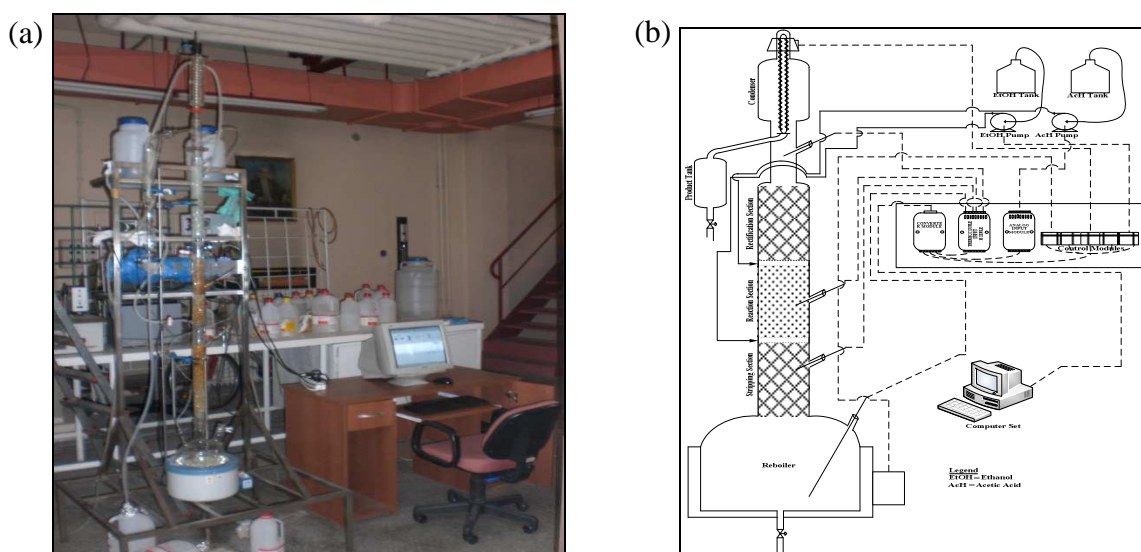
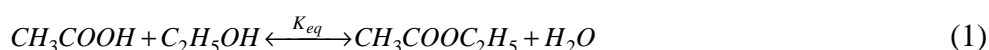


Figure 1: Reactive distillation column (a) Pictorial view; (b) Sketch view

2.2 Process Modeling Procedure:

The ethyl acetate reactive distillation process of this work was modeled in the form of state space models using System Identification Method by developing the state space models of the process with the aid of System Identification Toolbox of MATLAB (Ljung, 2012a; Ljung, 2012b) using the input-output data generated in the experiment 1 described in the work of Giwa and Karacan (2012e). Four different state space models were developed for the process. One of them was a continuous-time type while the remaining three were discrete-time types. The continuous-time type was developed using the *ssest* command while the discrete-time type models were developed using the *c2d*, *pem* and *n4sid* commands of MATLAB R2012a (Bemporad *et al.*, 2012a; Bemporad *et al.*, 2012b). The notations used to denote the models were derived from their MATLAB commands and they are as given in Table 1 below.

Table 1: Notations of the state space models

S/N	MATLAB command used	Notation
1	<i>ssest</i>	<i>ssest</i> model
2	<i>c2d</i>	<i>c2d</i> model
3	<i>pem</i>	<i>pem</i> model
4	<i>n4sid</i>	<i>n4sid</i> model

The form of the continuous-time state space model developed is given in Equation (2) as:

$$\left. \begin{aligned} \frac{dx}{dt} &= Ax(t) + Bu(t) + Ke(t) \\ y(t) &= Cx(t) + Du(t) + e(t) \end{aligned} \right\} \quad (2)$$

while that of the discrete-time state space model is as shown in Equation (3).

$$\left. \begin{aligned} x(t+Ts) &= Ax(t) + Bu(t) + Ke(t) \\ y(t) &= Cx(t) + Du(t) + e(t) \end{aligned} \right\} \quad (3)$$

where x is the state vector, u is the input vector and y is the output vector. A , B , C , D and K are the state space matrices used to express the process dynamics. They (A , B , C , D and K) can be regarded as the model coefficients and thus be called matrix model coefficients.

2.3 Control Simulation Procedure:

In the control aspect of this work, three controlled variables (top segment temperature (T_{top}), reaction segment temperature (T_{rxn}) and bottom segment temperature (T_{bot})) and three manipulated variables (reflux ratio (R), feed ratio (F) and reboiler duty (Q)) were selected for the formulation of the model predictive control algorithm. In addition, three (3) unmeasured disturbances (UDs) in forms of noise were also passed into the control system as part of the input variables. The algorithm was simulated with the aid of Model Predictive Control Toolbox of MATLAB (Bemporad *et al.*, 2012). The schematic form of the control system of this work is as shown in Figure 2 below.

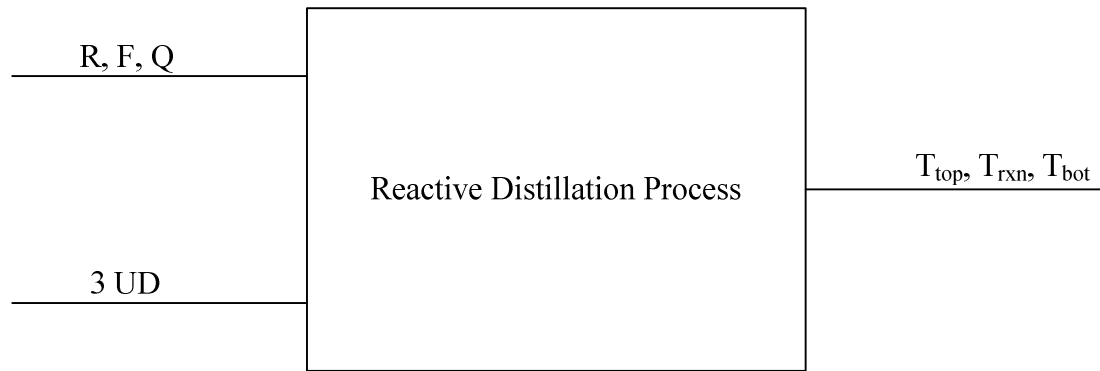


Figure 2: Model predictive control system for ethyl acetate reactive distillation process

The data used for the development of the control algorithm of the model predictive control of the reactive distillation process are as given in Table 2.

Table 2: Model predictive control algorithm formulation data

Description	Value
Sampling time (s)	1
Prediction horizon	11
Control horizon	7
Weights on manipulated variables	[0.00 0.00 0.00]
Weights on manipulated variables rate	[0.22 0.22 0.22]
Weights on output variables	[1.00 1.00 1.00]

3. Results and Discussion:

3.1 Process Modeling Studies:

The results obtained from the process identification studies are shown in the Table 3, 4, 5 and 6 below for the four different types of state space models developed.

Table 3: Model coefficients of *ssest* state space model

A			
	x ₁	x ₂	x ₃
x ₁	-0.0019	0.0024	-0.0009
x ₂	-0.0034	-0.0043	-0.0008
x ₃	-0.0009	-0.0052	-0.0055
B			
	u ₁	u ₂	u ₃
x ₁	0.0003	0.0013	-0.0566
x ₂	-0.0005	0.0019	-0.0822
x ₃	0.0025	0.0067	-0.2818
C			

	x_1	x_2	x_3
y_1	-12.8258	4.0787	0.1685
y_2	-3.7520	-0.8266	-1.9955
y_3	-6.2674	-17.6857	-0.7129
D			
	u_1	u_2	u_3
y_1	0.0000	0.0000	0.0000
y_2	0.0000	0.0000	0.0000
y_3	0.0000	0.0000	0.0000
K			
	y_1	y_2	y_3
x_1	-0.0440	-0.0058	-0.0114
x_2	0.0172	0.0046	-0.0430
x_3	0.0147	-0.1111	-0.0099

Table 4: Model coefficients of $c2d$ state space model

A			
	x_1	x_2	x_3
x_1	0.9981	0.0024	-0.0009
x_2	-0.0034	0.9957	-0.0008
x_3	-0.0009	-0.0052	0.9945
B			
	u_1	u_2	u_3
x_1	0.0003	0.0013	-0.0565
x_2	-0.0005	0.0019	-0.0818
x_3	0.0025	0.0067	-0.2808
C			
	x_1	x_2	x_3
y_1	-12.8258	4.0787	0.1685
y_2	-3.7520	-0.8266	-1.9955
y_3	-6.2674	-17.6857	-0.7129
D			
	u_1	u_2	u_3
y_1	0.0000	0.0000	0.0000
y_2	0.0000	0.0000	0.0000
y_3	0.0000	0.0000	0.0000

K			
	y_1	y_2	y_3
x_1	-0.0439	-0.0058	-0.0114
x_2	0.0172	0.0046	-0.0428
x_3	0.0146	-0.1108	-0.0098

Table 5: Model coefficients of *pem* state space model

A			
	x_1	x_2	x_3
x_1	0.9981	0.0024	-0.0009
x_2	-0.0034	0.9957	-0.0008
x_3	-0.0009	-0.0052	0.9946
B			
	u_1	u_2	u_3
x_1	0.0003	0.0013	-0.0563
x_2	-0.0005	0.0019	-0.0818
x_3	0.0025	0.0066	-0.2782
C			
	x_1	x_2	x_3
y_1	-12.8260	4.0786	0.1680
y_2	-3.7520	-0.8265	-1.9957
y_3	-6.2674	-17.6857	-0.7131
D			
	u_1	u_2	u_3
y_1	0.0000	0.0000	0.0000
y_2	0.0000	0.0000	0.0000
y_3	0.0000	0.0000	0.0000
K			
	y_1	y_2	y_3
x_1	-0.0439	-0.0057	-0.0114
x_2	0.0172	0.0046	-0.0428
x_3	0.0148	-0.1102	-0.0098

Table 6: Model coefficients of *n4sid* state space model

A			
	x_1	x_2	x_3
x_1	0.9972	0.0029	0.0003
x_2	-0.0059	0.9930	0.0003

x_3	-0.0012	-0.0062	0.9946
B			
	u_1	u_2	u_3
x_1	0.0002	0.0002	-0.0125
x_2	-0.0007	0.0016	-0.0697
x_3	0.0016	0.0066	-0.2779
C			
	x_1	x_2	x_3
y_1	-12.8264	4.0787	0.1688
y_2	-3.7502	-0.8260	-1.9960
y_3	-6.2676	-17.6857	-0.7126
D			
	u_1	u_2	u_3
y_1	0.0000	0.0000	0.0000
y_2	0.0000	0.0000	0.0000
y_3	0.0000	0.0000	0.0000
K			
	y_1	y_2	y_3
x_1	-0.0390	0.0041	-0.0085
x_2	0.0176	0.0081	-0.0310
x_3	0.0283	-0.0800	-0.0006

As can be observed from the model coefficients shown in the tables (Table 3, 4, 5 and 6) above, while some of the coefficients were positive, others were negative. The sign changes in the coefficients of the reactive distillation process could be attributed to the complex nature of the process. Apart from that, among the discrete models (those developed with *c2d*, *pem* and *n4sid* MATLAB commands), the coefficients of the *c2d* and that of *pem* state space models were found to be close to each other than to that of the *n4sid* model. This was the main reason why the dynamic behaviors of the *c2d* state space and that of *pem* state space models were discovered to be very similar in the control simulation studies discussed in the next section.

3.2 Control Simulation Studies:

The control studies of this work were simulated with the aim of raising the steady-state value of the top segment temperature from 69.89 °C to 70.75 °C. The temperature of 70.75 °C was found to be very important in the production of ethyl acetate from the esterification reaction between acetic acid and ethanol because, according to the information gathered from the literature, that was the temperature at which high composition of the desired product (ethyl acetate) could be achieved. In addition to applying a step to the top segment temperature steady-state value, steps of 0.5 and 1.5 °C were also applied to the steady-state temperatures of the reaction segment and the bottom segment temperatures respectively. The results obtained from the application of the steps are as shown in Figure 3, 4 and 5 respectively for the top segment, reaction segment and bottom segment temperature.

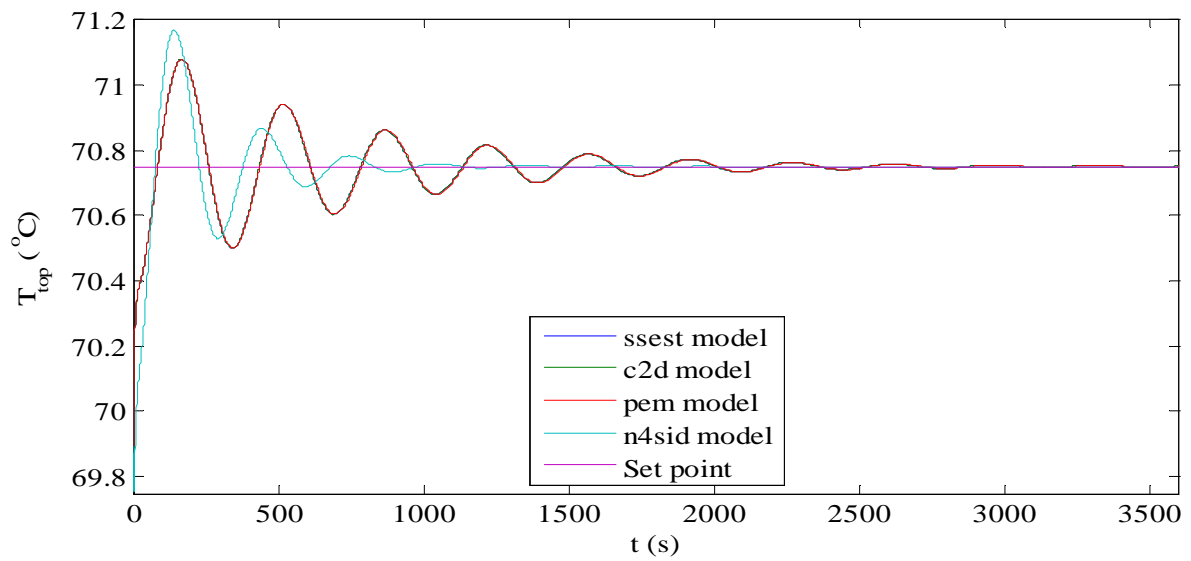


Figure 3: Dynamic responses of the control system to a 0.86 °C (from 69.89 to 70.75 °C) step in top segment temperature

From the results of the dynamic responses of the top segment temperature to the set-point change from 69.89 to 70.75 °C shown in Figure 3, as can be seen, even though the overshoot possessed by the *n4sid* state space model was the highest among the four state space models that were considered in this work, its dynamic behavior was found to have the lowest rise time and number of oscillations. In addition, the model (*n4sid* state space model) was discovered to settle fastest among the models. That is, it had the minimum response time. Also observed from Figure 3 was that the dynamic responses of the continuous-time state space model (*ssest* state space model) and those of the discrete-time state space models developed using the *c2d* and *pem* commands of MATLAB were very similar because their responses were even found to overlap.

Shown in Figure 4 are the dynamic responses of the reaction segment temperatures of the state space models to a 0.5 °C step in the reaction segment steady-state temperature value. From the figure, similar to what were observed in the case of the top segment temperature, the dynamic response of the *n4sid* state space model was found to give the highest overshoot but the lowest response time compared to the remaining state space models simulated.

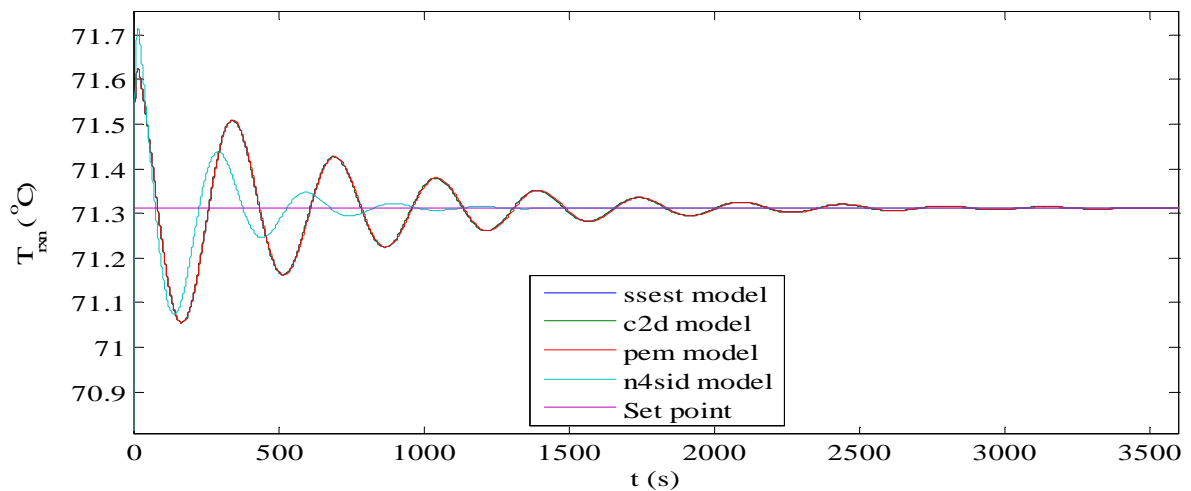


Figure 4: Dynamic responses of the control system to a 0.5 °C step in reaction segment temperature

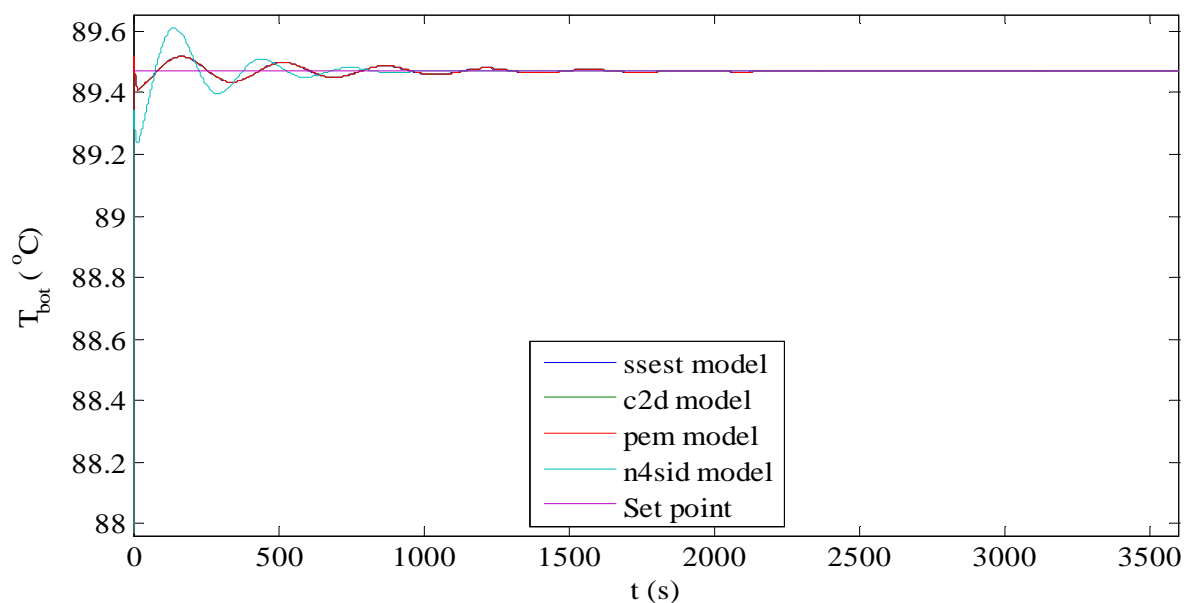


Figure 5: Dynamic responses of the control system to a 1.5 °C step in bottom segment temperature

The responses of the bottom segment temperature shown in Figure 5 above were also found to follow the same trend observed in the remaining two segment temperatures of the reactive distillation process as it could be discovered that, among the four state space models, the one with the lowest number of oscillations and response time was *n4sid* discrete-time state space model. As usual, the responses of the other two discrete-time state space (*c2d* and *pem*) models as well as that of the continuous-time state space (*ssest*) model were found to overlap.

After the simulation of the control system, the performance values of the control system towards each of the state space models were calculated. The performance criterion used in this study is the Integral Squared Error (ISE). The calculated values of the ISE for the four models simulated for the reactive distillation process control system are as given in Table 7.

Table 7: Control performance values

Control models	ISE values		
	T_{top}	T_{rxn}	T_{bot}
<i>ssest</i> model	1.14	0.50	2.26
<i>c2d</i> model	1.14	0.50	2.26
<i>pem</i> model	1.14	0.50	2.26
<i>n4sid</i> model	1.08	0.36	2.29

As can be seen from Table 7, the Integral Squared Error values calculated for the *ssest*, *c2d* and *pem* state space models were found to be approximately the same and have the values of 1.14, 0.50 and 2.26 while those of the *n4sid* state space model were found to be 1.08, 0.36 and 2.29 respectively for the top segment temperature, reaction segment temperature and bottom segment temperature. The performance values (as seen in Table 7) of the controllers developed with the four state space models were discovered to be good (low) enough to say that the controllers had very high performances for set-point tracking.

Comparing their performances, the *n4sid* state space model can be said to be the best among the state space models considered because, apart from the fact that it produced the dynamic responses with the lowest number of oscillations and response time, its Integral Squared Error for two different segment temperatures were found to be the lowest compared to those of the other state space models. As such,

it was chosen as the state space model used in describing the dynamics of the reactive distillation process for process model mismatch studies.

In the mismatch studies, new plant models having gains of 20% and 40% larger than those in the original *n4sid* state space model were used in the controller and the simulations of the control system were repeated. The results of the mismatch simulations are as shown in Figure 6, 7 and 8 for the top segment, reaction segment and bottom segment temperatures respectively. As can be observed from the figures (Figure 6 – 8), as the mismatch was increasing, the overshoot was also increasing. However, the rise time was found to decrease with increase in the mismatch but the response times of the all the simulations (with and without mismatch) carried out for the reactive distillation process were found to be approximately the same and about 1000 s.

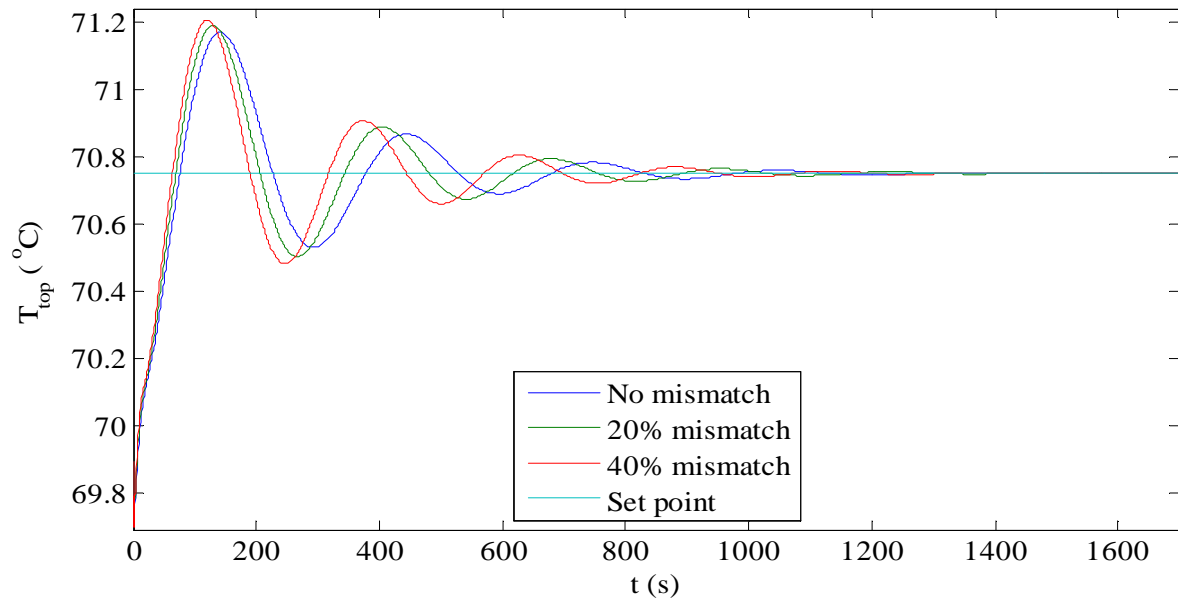


Figure 6: Dynamic responses of the control system to a 0.86 °C (from 69.89 to 70.75 °C) step in top segment temperature with and without mismatches

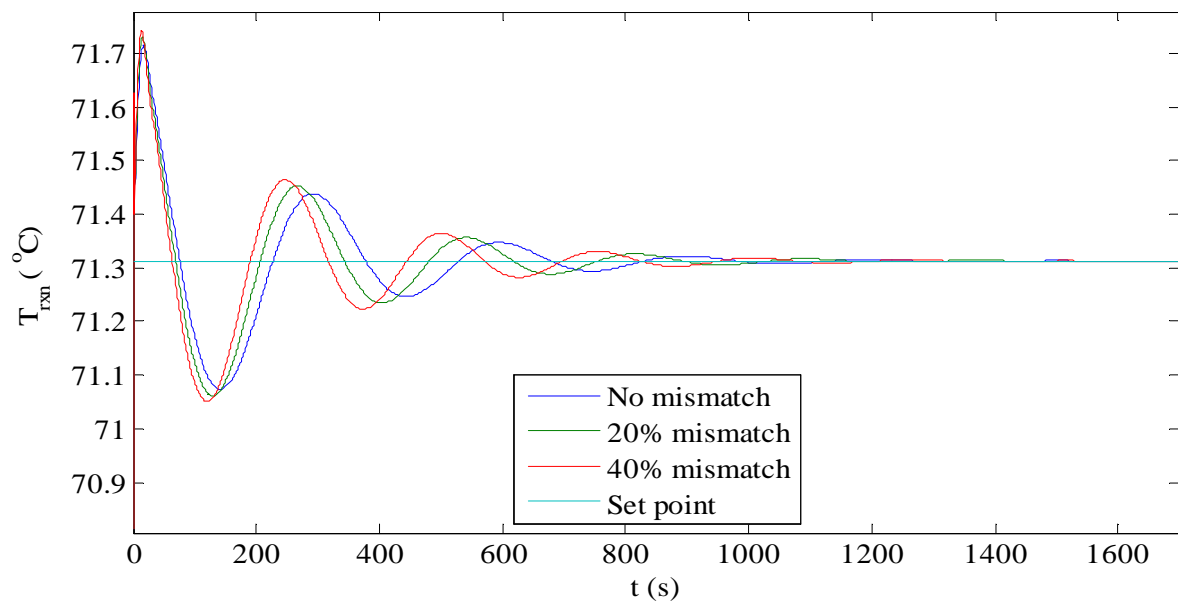


Figure 7: Dynamic responses of the control system to a 0.5 °C step in reaction segment temperature with and without mismatches

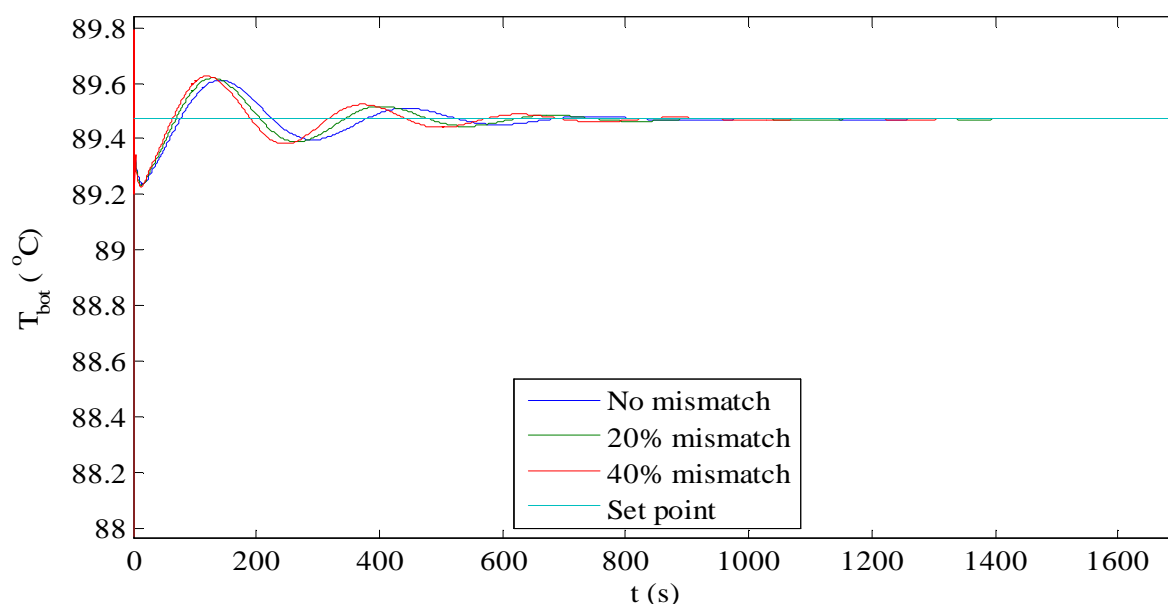


Figure 8: Dynamic responses of the control system to a 1.5 °C step in bottom segment temperature with and without mismatches

The similarity in the approximate response times of the plant models with and without mismatch was an indication of the fact that the mismatch did not affect the performance of the controller seriously. In other words, the controller developed using the *n4sid* state space model was found to be robust because it was able to produce satisfactory performance even in the presence of some degrees of model inaccuracy.

4. Conclusions:

The results obtained from the simulations of model predictive control system using four different state space models of the reactive distillation process used for the production of ethyl acetate have revealed that the Integral Squared Error of the top segment and reaction segment temperatures of the control system formulated using the *n4sid* state space model were lower than those of the other models. Therefore, it was concluded that *n4sid* state space model was able to produce the best closed-loop dynamic response among the models investigated and it was thus selected as the best state space reactive distillation process model that was used and that can still be used for further investigation in the control studies.

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Nomenclatures

F	Feed ratio (mL s^{-1} of acetic acid feed rate / mL s^{-1} of ethanol feed rate)
ISE	Integral Squared Error
MATLAB	Matrix Laboratory

MPC	Model Predictive Control
Q	Reboiler duty (kJ/s)
R	Reflux ratio
RDP	Reactive Distillation Process
t	Time (s)
T _{bot}	Bottom segment temperature (°C)
T _{rxn}	Reaction segment temperature (°C)
T _{top}	Top segment temperature (°C)
UD	Unmeasured disturbance

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